

Cumene  
98-82-8 | DTXSID1021827

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:** 1.20e-10 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:** 2.89e-01

**Confidence level:** 9.09e-01

## Nearest Neighbors from the Training Set

Image not found

1,3,5-Cycloheptatriene

**Measured:** 9.69e-11

**Predicted:** 1.00e-10

Image not found

Cyclohepta-1,3-diene

**Measured:** 1.39e-10

**Predicted:** 1.35e-10

Image not found

1,4-Cyclohexadiene

**Measured:** 1.00e-10

**Predicted:** 1.11e-10

Image not found

2,5-Norbornadiene

**Measured:** 1.20e-10

**Predicted:** 1.20e-10